



Late-Combustion Soot Burnout Investigated

The understanding of diesel combustion and emissions formation has been advanced considerably in recent years by the application of advanced laser diagnostics. However, previous studies have generally focused on the early and middle stages of diesel combustion, and there is little detailed understanding of the late stages and the mechanism whereby soot escapes oxidation to become a tail-pipe emission. John Dec and Peter Kelly-Zion have been investigating late-combustion soot burnout in a firing diesel engine by simultaneously imaging the OH-radical and soot distributions using planar laser-induced fluorescence (PLIF) and planar laser-induced incandescence (PLII), respectively.

Measurements were made in an optically accessible direct-injection (DI) diesel engine of the heavy-duty size class, derived from a Cummins N-series production engine. A dual-laser, dual-camera system was used to obtain the simultaneous "single-shot" images (see Fig 1). The OH PLIF laser was tuned to a strong feature of the A-X, (1,0) transition at 284.01 nm, and a frequency-doubled Nd:YAG laser (532 nm) was used to create the PLII signal. The two laser beams were combined into

overlapping laser sheets and directed into the combustion chamber. Images were acquired through the piston-crown window with the OH and soot signals being separated into the two intensified video cameras by means of an edge filter. Each camera was equipped with additional filters to isolate the appropriate signal.

During the late stages of diesel combustion, OH radicals were found to occur in the remaining diffusion flame zones and the hot post-combustion gases. Because OH occurs only in these hot-gas regions, and because OH-radical attack is considered to be the main mechanism for soot oxidation, the OH radical distribution is a particularly good marker of regions where soot oxidation can occur. PLII soot-distribution images show where soot remains during the late stages of diesel combustion, and simultaneous images of soot and OH show their relative locations, allowing the potential for oxidation of the remaining soot to be assessed.

Temporal sequences of simultaneous soot and OH images were obtained during the late stages of diesel combustion for several laser-sheet elevations and for various injection timings, engine speeds, fuel loadings, and diluent levels. Two of these images are shown in Fig. 2. The image sequences show the progression of the soot and OH distributions during the burnout period for each condition. Comparisons of these sequences provide substantial insight into the changes that occur to the soot burnout in the bulk gas as operating conditions are changed.

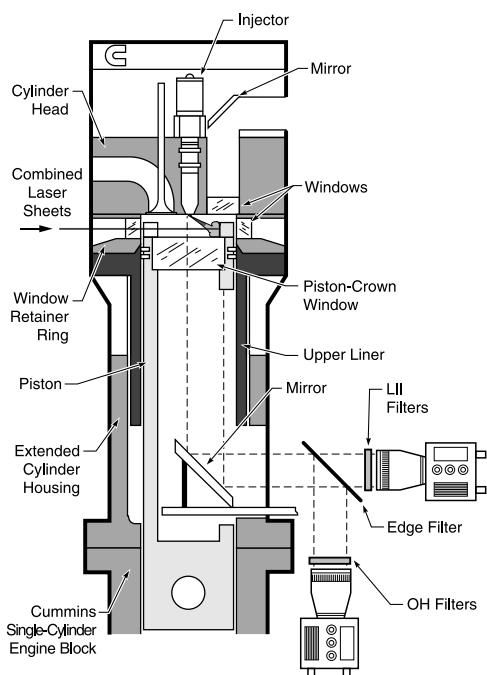


Figure 1. Schematic of the optically accessible heavy-duty diesel engine, showing the orientation of the combined laser sheets and the location of the cameras.

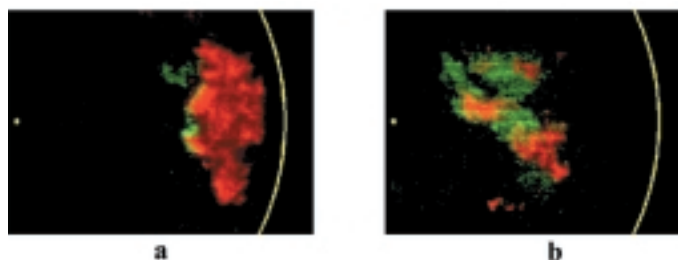
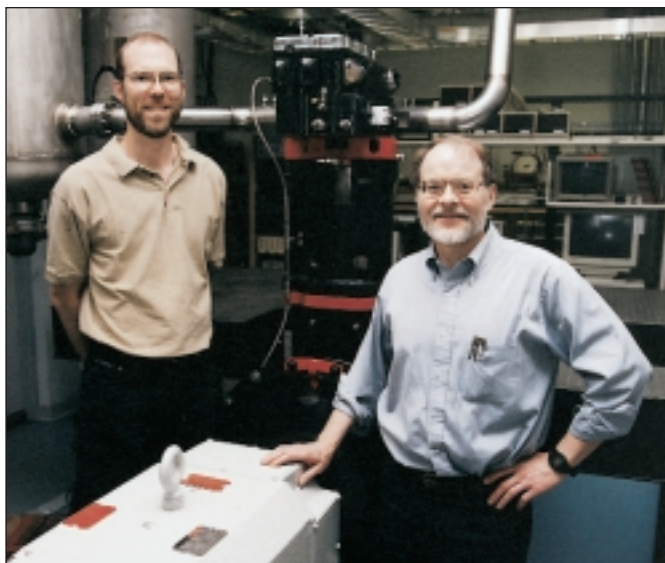


Figure 2. Simultaneous PLIF-OH and PLII-soot images at two times during the late-combustion soot burnout. The OH and soot images are superimposed and shown as green and red, respectively, with the overlap regions shown in yellow. The small yellow dot at the left shows the location of the injector, and the yellow curve at the right indicates the location of the edge of the combustion bowl when the piston is near TDC, as shown in Fig. 1. Image "a" is typical of the early part of the burnout period, and image "b" shows soot oxidation continuing after the end of the apparent heat release.



Peter Kelly-Zion (left), a post-doctoral appointee, has spent the past year working with John Dec in the Heavy-Duty Diesel Engine Combustion Laboratory. Peter has worked mainly on two projects: 1) an investigation of late-combustion soot burnout in the diesel engine, using simultaneous imaging of the OH radical and soot (article in this CRF News), and 2) kinetic-rate computations of compression-induced autoignition of higher hydrocarbons, using CHEMKIN with detailed chemistry from LLNL. Peter has accepted a faculty position at Trinity University in San Antonio starting this fall.



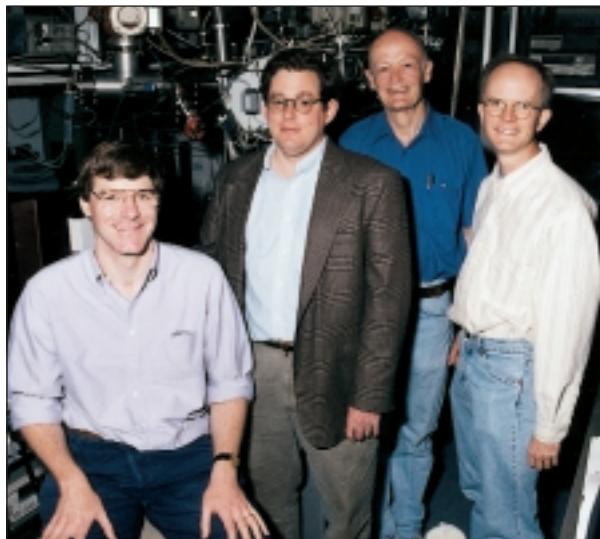
Michael Di Rosa (left) has recently completed a three-year term as a Sandia post-doctoral appointee, working with Roger Farrow. Mike and Roger have been investigating two-photon excitation methods for detecting carbon monoxide in combustion environments.

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CRF Phase II Formal Opening

With the successful completion of the construction project last year and specialization and equipping of the last of the remaining new laboratories this year, we are planning a formal opening of the Phase II laboratory addition in the Fall of 1999. Although plans are not yet finalized, our targeted date is November 18th. Stay tuned for more information and a firm date to be announced in the next issue of the CRF News.



Terry Cool from Cornell University, Charles Pibel from American University, and Jay Thoman from Williams College have just completed several projects with Andy McIlroy. Terry has made species profile measurements in low-pressure dimethylether flames using the photoionization mass spectrometer that he has helped develop at Sandia. Charles has extended his studies of vinyl radical electronic spectroscopy using the cavity ringdown technique in both room temperature photolysis flow cell and molecular beam discharge sources. Jay has developed a cavity ringdown technique for measuring space resolved, absolute CH number densities in low-pressure flames. From left: Jay Thoman, Charles Pibel, Terry Cool, and Andy McIlroy.



Wolfgang Meier (DLR Stuttgart, Germany, left) and Rob Barlow conducted a backyard review of Rayleigh/Raman/LIF measurements obtained in turbulent jet flames of $\text{CH}_4/\text{H}_2/\text{N}_2$ burning in air. Wolfgang collaborated with Rob and Ying-Ling Chen in the Turbulent Diffusion Flame lab during his six-week visit to the CRF.

Sodium Species Measured in Glass Melting Furnaces

During the last decade there has been a marked increase in the use of oxygen in place of air for combustion of natural gas in glass melting furnaces, to reduce emissions of NO_x and particulate matter and to improve efficiency. For reasons not well understood, firing with oxygen appears to accelerate corrosion of the refractory crown (roof) in some glass melting furnaces. Corrosion is due to the reduction in melting temperature of silica refractory following its reaction with sodium atoms and sodium hydroxide, which vaporize from the glass into the combustion products. Contributing to sodium vaporization are higher flame temperatures, longer gas residence times, and higher concentrations of water vapor when firing with oxygen. In addition to their role in refractory corrosion, the sodium species are converted to sodium sulfate as the exhaust cools and are the principal source of particulate matter in the flue gas. If the vaporization and transport of sodium are to be controlled, one must first be able to observe and measure it.

Sandians Bob Gallagher, Peter Walsh, Neal Fornaciari, Steve Buckley (now at the University of Maryland), David Hahn (now at the University of Florida), Howard Johnsen, Jimmy Ross, and Ed Walsh began work on the measurement of sodium in 1997, in collaboration with John Brown, Mahendra Misra, Fred Quan, and Steve Tong of Corning Incorporated, Vince Henry and Kanwal Bhatia of Visteon Glass Systems, and Doug Moore, Lance Lemings, John Neufeld, and Dennie Lowe of the

Gallo Glass Co., with financial support from Corning, Visteon, and DOE/Office of Industrial Technologies. Measurements were made at Gallo Glass in the first large furnace converted from air to oxygen firing by a team led by Doug Moore and John Brown.

Concentrations of sodium atoms, integrated over the line-of-sight across the furnace, were measured by Peter Walsh, in collaboration with Phil Paul, using emission and absorption of light in the far wings of the sodium D-lines. The total sodium mole fraction, assuming that the gaseous species were in equilibrium, was typically 100 to 200 ppm, of which 10 to 60% were sodium atoms. Other alkali metals, lithium, potassium, and rubidium, were also observed in the emission spectrum, and are expected to contribute to refractory corrosion.


Steve Buckley, David Hahn, Howard Johnsen, and Jimmy Ross took a different approach, making measurements in the flue downstream from the furnace using laser-induced breakdown spectroscopy (LIBS) to determine the total sodium in the combustion products. The portable LIBS probe, shown in Figure 1, focuses the output from a pulsed Nd:YAG laser (1064 nm) in the flue gas. Electric breakdown at the focal point generates a plasma, vaporizes particles, dissociates the gas and vapor, and excites the atoms. The wavelengths and intensities of atomic lines in the emission spectrum identify the elements present and, with appropriate calibration, their concentrations. Measurements of sodium in the flue during a six-hour period are shown in Figure 2. The mole fractions, 60 ± 10 ppm, were lower than in the furnace, because the flue gas is diluted with air and quenched by injection of water. The difference in average sodium levels at the beginning and end of the record suggests an opportunity for some degree of control. Response of sodium to changes in furnace conditions will be examined in future work. 



Figure 1. Portable Laser-Induced Breakdown Spectroscopy (LIBS) instrument package mounted on the flue duct at the Gallo Glass Co., Modesto, California. A Nd:YAG laser is inside the gray box just below and to the right of center. To its left, the delivery and collection optics are housed in the black unit and steel tube sealed into the wall of the horizontal flue duct.

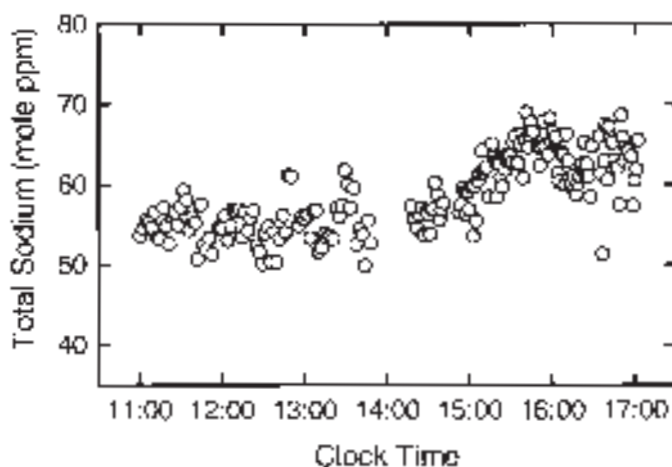



Figure 2. Total sodium mole fraction in the flue gas as a function of time.

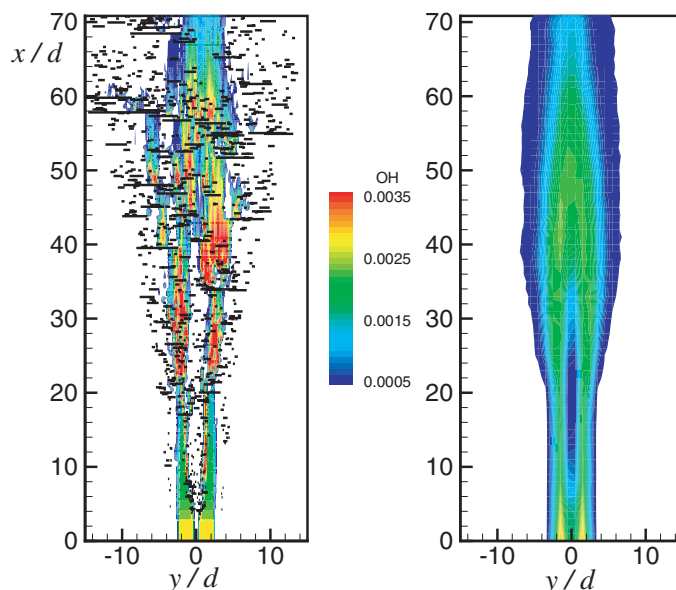
Structure of Turbulent Diffusion Flames Revealed Using a Novel Turbulence Model

Tarek Echekki, Alan Kerstein, and J.-Y. Chen (U. C., Berkeley) have recently developed a new formulation for turbulent diffusion flames based on the novel One-Dimensional Turbulence (ODT) model. ODT involves a new turbulence modeling strategy that captures key mechanisms of multidimensional turbulent flow with a one-dimensional description (CRF News 18:3). Tarek, Alan, and J.-Y. extended this formulation to turbulent reacting flows by coupling the model to Sandia's CHEMKIN chemical-kinetics package. The resulting formulation is fully resolved in time and in space (on the 1D domain) and captures relevant fine scale processes that govern the so-called turbulence-chemistry interactions.

The figure shows illustrative results of computations of piloted methane-air jet diffusion flames that were performed using the model. The flame conditions correspond to a recent Sandia experiment by Robert Barlow and Jonathan Frank (CRF News 20:2). The OH concentration field from a single realization is compared to an averaged field. The single realization is characterized by spatial fluctuations that result from the combined contributions of stirring and chemistry. The average reflects pilot-assisted burning up to twenty diameters downstream, followed by self-sustained burning fed by air entrained from the coflow.

The rendering of stirring events shows that the model reproduces a number of known features of turbulent shear flow structure. The onset of turbulence along the fluid interfaces of highest shear (i.e., the shear layers where the inner flow meets the slower pilot flow, and where the pilot flow meets the weak outer flow) is evident. Between the high-shear regions, the nonturbulent core of the inner jet and of the pilot flow is delineated. (This simulation assumes laminar inflow, but turbulent inflow can also be simulated.) Farther downstream, the merging of these regions, the onset of a 'turbulent cascade' (with smaller eddies trailing larger ones) and associated 'spatial intermittency' are seen.

The team has shown that the model, with minimal empiricism, yields good predictions of means and fluctuations of the thermochemical scalar fields as seen in diffusion flame measurements performed at the CRF and elsewhere. Applications of the present formulation to flames in stagnating turbulence and to autoignition are also anticipated. 



Two-dimensional renderings (smoothed for clarity) of the OH mass-fraction field for a single realization (left) and for an average of 100 simulations (right) of a piloted methane-air diffusion flame. Also shown on the single realization is a rendering of stirring events (horizontal line segments) that represent turbulent eddies in the simulation. The 1D domain corresponds to the y axis (scaled by inner-flow diameter d). Its temporal evolution is converted to downstream distance from the jet inlet, corresponding to the x axis (scaled by d).



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